

Calculating critical temperatures of superconductivity from a renormalized Hamiltonian

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Abstract. – It is shown that one can obtain quantitatively accurate values for the superconducting critical temperature within a Hamiltonian framework. This is possible if one uses a renormalized Hamiltonian that contains an attractive electron–electron interaction and renormalized single particle energies. It can be obtained by similarity renormalization or using flow equations for Hamiltonians. We calculate the critical temperature as a function of the coupling using the standard BCS–theory. For small coupling we rederive the McMillan formula for T_c . We compare our results with Eliashberg theory and with experimental data from various materials. The theoretical results agree with the experimental data within 10%. Renormalization theory of Hamiltonians provides a promising way to investigate electron–phonon interactions in strongly correlated systems.

Introduction. – For more than three decades Eliashberg theory [1] has been the standard theory to compute quantitative properties of superconductors like the critical temperature. For a review we refer to [2, 3]. The basic advantage of Eliashberg theory compared to BCS–theory [4] is that it provides a framework to treat real phonon spectra and strong electron–phonon coupling. The critical temperature of a superconductor can be calculated with great accuracy [5]. Eliashberg theory is based on a description in terms of Green’s functions. It becomes exact in the limit where the electron mass is small compared to ion masses.

In the past ten years, several new developments like the discovery of high- T_c materials [6] and heavy fermions (for a recent theoretical review see [7]) stimulated research activities in strongly correlated systems [8]. Theories of strongly correlated systems are usually based on a Hamiltonian description, which is the natural basis to investigate properties of bound states. If one wants to investigate the effect of the electron–phonon interaction in strongly correlated systems, one has to set up a model Hamiltonian that contains phononic degrees of freedom. The main problem is that the standard Eliashberg theory cannot be applied to such models, because it cannot be formulated in a Hamiltonian framework. There are also other difficulties, for instance in heavy fermion systems, where the mass of the quasi-particles becomes comparable

to the ion masses, so that Eliashberg theory is no longer applicable. Despite years of effort, our understanding of electron–phonon interactions in strongly correlated systems is rather poor. The major problem is that one needs a theoretical method based on a Hamiltonian description that allows an accurate treatment of the electron–phonon interaction.

BCS–theory is based on a Hamiltonian approach, but it does not contain the electron–phonon interaction explicitly. Most of the properties of superconductors can be understood using BCS–theory. But one of the problems of BCS–theory is that the characteristic energy scale that determines the critical temperature T_c of the superconductor or the gap cannot be calculated. The famous BCS–formula $T_c = 1.13\Theta \exp(-1/N(\epsilon_F)V)$, where Θ is the Debye temperature and V is the strength of the interaction, has to be used to determine the parameter $N(\epsilon_F)V$ from T_c . Usually it is argued that the problems of BCS–theory are due to the fact that retardation effects in the interaction are neglected [3]. This viewpoint is possible if one has a theory in terms of Green’s functions in mind like the Eliashberg–theory. In a Hamiltonian framework one usually works with instantaneous interactions. From a viewpoint based on a Hamiltonian the problem of BCS–theory is that the effective Hamiltonian has to be obtained from an initial Hamiltonian containing electrons and phonons. The effective electron–electron interaction Bardeen *et al.* [4] had in mind was the phonon–induced interaction of Fröhlich [9] or Bardeen and Pines [10]. These interactions are constructed perturbatively. But regarding the energy scales in the problem it is clear that a perturbative approach must fail. The initial Hamiltonian is dominated by the electronic energies, which are typically of the order of a few eV. Further it contains phonons with an energy scale of the order 10meV. Superconductivity arises due to a marginal relevant operator, the phonon–induced electron–electron interaction. The relevant energy scale in this problem is set by the critical temperature, which is typically at least an order of magnitude smaller than the phonon energies. Thus, if one wants to obtain accurate values for the critical temperature, one has to resolve an energy scale which is about five orders of magnitude smaller than the typical energy scale in the initial Hamiltonian. This means that one needs a renormalization procedure which allows to calculate an effective renormalized Hamiltonian from the initial Hamiltonian to high accuracy.

Construction of the renormalized Hamiltonian. – A general renormalization procedure for Hamiltonians has not been available for long time, although in his first paper on renormalization Wilson treated a Hamiltonian problem [11]. The only accurate renormalization procedure for Hamiltonians was numerical renormalization, which could be applied to fermionic single impurity problems. Three years ago, a new method for calculating effective Hamiltonians has been proposed by Wegner [12]. It uses continuous unitary transformations to calculate an effective Hamiltonian from a given initial one. This method has been called *flow equations for Hamiltonians*. It has been applied successfully to single impurity problems [13] and to dissipative quantum systems [14]. Independently of Wegner, Glazek and Wilson [15] proposed a similar method, *similarity renormalization*. They use continuous unitary transformations to renormalize a given Hamiltonian. The aim of Wilson *et al.* is to treat light–front QCD [16]. Recently Brisudová *et al.* calculated quarkonium spectra using this method [17]. Both methods have a large range of possible applications in many particle physics. The aim of this work is to show that reliable quantitative results can be obtained with the framework of renormalization of Hamiltonians.

Both methods, flow equations and similarity renormalization, have been applied to the electron–phonon problem [18, 19]. Lenz and Wegner used the flow equations to calculate the effective electron–electron interaction. Their result differs significantly from the one obtained by Fröhlich [9] or Bardeen and Pines [10]. The interaction within a Cooper pair they obtained has no singularity and is attractive in the whole parameter space. In [19] I applied the similarity renormalization scheme to the electron–phonon problem. The effective interaction one obtains

is similar to the one calculated by Lenz and Wegner. Furthermore, the single particle energies in the original Hamiltonian are renormalized. I calculated the critical temperature for a simple Einstein model. The aim of the present work is to show that T_c can be calculated for realistic phonon spectra using this method. The results agree very well with results from Eliashberg theory and with experimental data.

Our starting point is the standard Hamiltonian for the electron–phonon problem

$$H = H_0 + H_I \quad (1)$$

with

$$H_0 = \sum_k \epsilon_k : c_k^\dagger c_k : + \sum_q \omega_q : b_q^\dagger b_q :, \quad (2)$$

$$H_I = \sum_{k,q} (g_{k,q} c_k^\dagger c_{k+q} b_q^\dagger + g_{k,q}^* c_{k+q}^\dagger c_k b_q). \quad (3)$$

c_k^\dagger and c_k are the creation and annihilation operators for electrons. I have not included spin and band indices, but this can be done without difficulty. b_q^\dagger and b_q are the creation and annihilation operators for phonons, here as well different acoustical and optical branches can be introduced. The colons denote normal ordering. In [19] I showed how this problem can be treated using similarity renormalization. The basis of this approach is a continuous unitary transformation applied to the Hamiltonian. The transformation can be written in the form $dH_\lambda/d\lambda = [\eta_\lambda, H_\lambda]$. λ is a ultra-violet cutoff, and the generator η_λ is chosen so that off-diagonal matrix elements vanish in H_λ if the corresponding energy difference is larger than λ . Details of this method in the present context are explained in [19], a general description can be found in [15, 16]. During the transformation the electron–phonon coupling is eliminated successively and an effective electron–electron interaction is generated. The final result is an effective Hamiltonian that contains an electronic part of the form

$$H_{\text{el}}^r = \sum_k \epsilon_k^r : c_k^\dagger c_k : - \frac{1}{2} \sum_{k,k',q} V_{kk'q} : c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k :, \quad (4)$$

a part describing the phononic degrees of freedom and a weak electron–phonon coupling. The remaining electron–phonon coupling contains a small part of the initial electron–phonon coupling and other couplings involving two or more phonons. In [19] these couplings have been neglected since they are of higher order in the coupling constant $g_{k,q}$. In principle it is possible to eliminate these couplings as well. This yields an additional contribution to the induced electron–electron interaction that is also of higher order.

Gap and critical temperature. – In the following we will analyse the properties of the electronic subsystem described by the renormalized Hamiltonian (4) using BCS–theory. To do this we use the well known BCS gap equation

$$\Delta_k = \sum_q \frac{V_{k,-k,q} \Delta_{k+q}}{2\sqrt{\epsilon_{k+q}^r{}^2 + \Delta_{k+q}^2}} \tanh \left(\frac{\beta}{2} \sqrt{\epsilon_{k+q}^r{}^2 + \Delta_{k+q}^2} \right). \quad (5)$$

It contains the interaction $V_{k,-k,q}$ of two electrons forming a Cooper pair. In standard BCS–theory this interaction is often approximated by a constant in a small energy interval around the Fermi surface. The result of Fröhlich [9] for this interaction is attractive in a small region around the Fermi surface, it has a divergency due to a vanishing energy

denominator and becomes repulsive in the rest of the parameter space. In contrary, the result by Lenz and Wegner [18] is attractive in the whole parameter space, it is of the form $V_{k,-k,q} = |g_{k,q}|^2 \omega_q / ((\epsilon_k - \epsilon_{k+q})^2 + \omega_q^2)$. Similarity renormalization yields a similar result, $V_{k,-k,q} = |g_{k,q}|^2 / (|\epsilon_k^r - \epsilon_{k+q}^r| + \omega_q)$ [19]. In the isotropic case, and introducing the renormalized density of states $N(\epsilon)$, the sum in (5) can be replaced by an integral. Furthermore, the electron-phonon coupling can be described by the standard Eliashberg function $2\alpha^2 F(\omega)$ [2]. The gap equation can then be written in the form

$$\Delta(\epsilon) = \int d\epsilon' \frac{N(\epsilon') \Delta(\epsilon')}{2\sqrt{\epsilon'^2 + \Delta(\epsilon')^2}} \tanh\left(\frac{\beta}{2} \sqrt{\epsilon'^2 + \Delta(\epsilon')^2}\right) \frac{1}{N(\epsilon_F)} \int_0^\infty d\omega \frac{2\alpha^2 F(\omega)}{|\epsilon - \epsilon'| + \omega}. \quad (6)$$

The factor $1/N(\epsilon_F)$ is due to the definition of $\alpha^2 F(\omega)$, which contains a factor $N(\epsilon_F)$. As a further approximation we replace the electronic density of states $N(\epsilon)$ by a constant N_0 . Since the electronic energies that enter in (5) are renormalized, this has to be taken into account. As in Eliashberg theory [2], similarity renormalization yields a renormalization of the electron energies $\epsilon_k^r = \epsilon_k / (1 + \lambda)$ [19] close to the Fermi surface. Therefore the renormalized density of states $N(\epsilon_F)$ at the Fermi surface can be replaced by $N(\epsilon_F) = N_0(1 + \lambda)$. λ is the usual coupling strength in the theory of superconductivity, defined as $\lambda = \int_0^\infty d\omega 2\alpha^2 F(\omega) / \omega$. In a first step we use (6) to determine T_c for weak coupling. If T is close to T_c , one can replace $\sqrt{\epsilon'^2 + \Delta(\epsilon')^2}$ by $|\epsilon'|$. We let $\epsilon = 0$ and use that $\Delta(\epsilon') \int_0^\infty d\omega 2\alpha^2 F(\omega) / (\epsilon' + \omega)$ is bounded, monotonic decreasing, and nonnegative. The second mean value theorem then yields

$$\frac{\lambda}{1 + \lambda} \int_0^{\tilde{\omega}} d\epsilon \tanh(\epsilon/2T_c) / \epsilon = 1. \quad (7)$$

Keeping the leading logarithmic singularity this yields $T_c \propto \tilde{\omega} \exp(-(1 + \lambda)/\lambda)$. $\tilde{\omega}$ can be obtained if one uses the second mean value theorem for $\tanh(\epsilon/2T_c)$ and for $\Delta(\epsilon)$. Then one obtains $\tilde{\omega} \propto \omega_{\log}$; $\omega_{\log} = \exp(\langle \ln \omega \rangle)$, where the average $\langle \ln \omega \rangle$ is taken with respect to the weight function $\alpha^2 F(\omega) / \omega$. Taking into account that the density of states $N(\epsilon)$ is not constant, one can introduce an additional constant in the argument of the exponential function. In this way one obtains a T_c equation of the form

$$T_c = c' \omega_{\log} \exp(-c \frac{1 + \lambda}{\lambda}). \quad (8)$$

It has the same form as the McMillan equation [20]. For small coupling ($\lambda < 1$) T_c / ω_{\log} does not depend on the details of the phonon spectrum; this has also been shown in the framework of Eliashberg theory [5].

In order to obtain results for T_c which can be compared with experimental data, one has to include the Coulomb repulsion. In principle this can be done from the very beginning. For our purpose it is sufficient to include the pseudo Coulomb potential [3, 2] μ^* by hand. With the assumption of a constant density of states the gap equation (6) can then be written as

$$\Delta(\epsilon) = \int d\epsilon' \frac{\Delta(\epsilon')}{2\sqrt{\epsilon'^2 + \Delta(\epsilon')^2}} \tanh\left(\frac{\beta}{2} \sqrt{\epsilon'^2 + \Delta(\epsilon')^2}\right) \frac{1}{1 + \lambda} \left(\int_0^\infty d\omega \frac{2\alpha^2 F(\omega)}{|\epsilon - \epsilon'| + \omega} - \mu^* \right). \quad (9)$$

For small coupling one can again derive a McMillan-type formula. For small λ the critical temperature does not depend on the details of $\alpha^2 F(\omega)$, but only on ω_{\log} . To obtain accurate

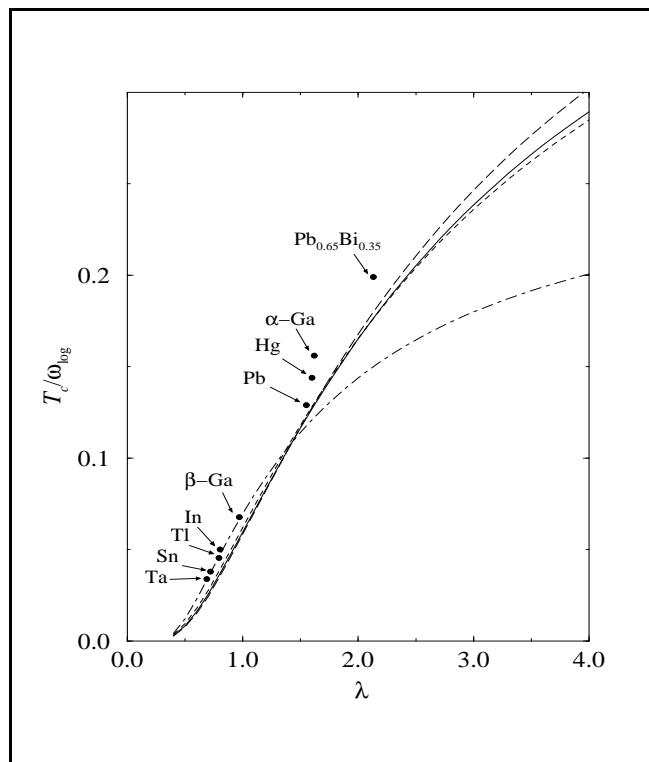


Fig. 1. – T_c/ω_{\log} plotted versus λ for $\mu^* = 0.1$ and various types of spectra. The solid line is calculated for a lead-type spectrum, the long-dashed line for a mercury like spectrum, and the short dashed line for an Einstein spectrum. Also included is the McMillan curve (dot-dashed) and some experimental data.

results, the gap equation (9) has to be solved numerically for a given form of the phonon spectrum. In Fig. 1 we show numerical results for T_c in units of ω_{\log} as a function of λ for various types of spectra and $\mu^* = 0.1$. The solid curve is the results for a spectrum of lead. Here $\alpha^2 F(\omega)$ can be well approximated by a suitable sum of Lorentzians [2]. This has the advantage that the ω -integral in (9) can be calculated analytically. The remaining integral can easily be calculated numerically to obtain T_c . The dotted curve is the result for an Einstein spectrum and has already been shown already in [19]. The dashed curve shows the result for a spectrum of mercury type. We have chosen these spectra since Allen and Dynes [5] calculated T_c for the same spectra in the framework of Eliashberg theory. This allows a direct comparison with Eliashberg theory. The corresponding curves lie slightly above our results, the difference is about 5%. We have included in our plot some experimental data also shown in [5]. A similar calculation can be done using the effective phonon-induced electron–electron interaction obtained by Lenz and Wegner [18]. The curves differ about 2% from the curves shown in Fig. 1. For the Einstein model, this has already been observed in [19]. One notices that our results are systematically a few percent too small compared to the results from Eliashberg theory or to experimental data. The reason is probably that we neglected higher order terms in the effective Hamiltonian that describe an interaction between electrons and two phonons. Treating these terms in the same way as the electron–phonon interaction, one obtains an additional contribution to the effective electron–electron interaction, which is of

fourth order in the initial electron–phonon coupling. This contribution is again attractive and will lead to a somewhat higher value of the critical temperature.

Conclusions. – Our result shows that similarity renormalization or flow equations for Hamiltonians yield an effective Hamiltonian that contains the correct energy scale. The quantitative results are comparable to Eliashberg theory. But these methods work in a Hamiltonian framework, using continuous unitary transformations, and they do not rely on special properties like a small ratio of electron mass to ion masses. Therefore one may hope that the analytical treatment of electron–phonon interactions in strongly correlated systems is as well possible using these methods.

From the viewpoint of Eliashberg theory or of a field theoretical approach based on a Lagrangian, where the phonons can be integrated out explicitly, a problem may still be that the effective interaction we calculated contains no retardation effects. But it should be pointed out that a quantity like T_c or the energy gap is not a dynamical quantity, but a spectral property of the Hamiltonian. Dynamical correlation functions of some observable can be calculated as well using continuous unitary transformations. One has to take the transformation of the observable into account. This has been shown in a recent investigation of dissipative quantum systems in a Hamiltonian framework [14]. Using flow equations for Hamiltonians one can obtain accurate quantitative results for dynamical low temperature correlation functions as well.

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